PATENT ABSTRACTS OF JAPAN

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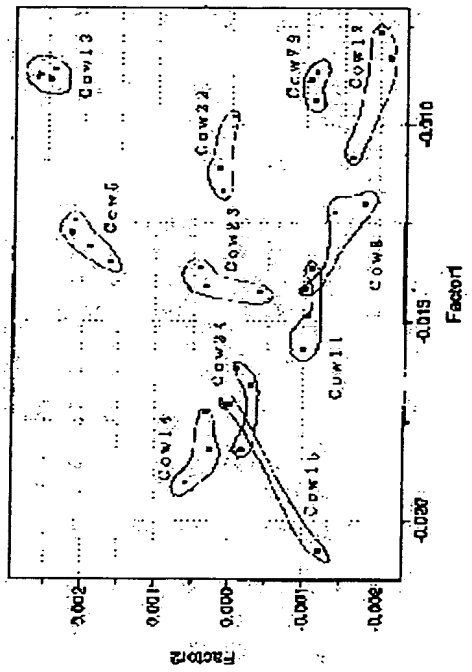
(54) METHOD FOR ACQUISITION OF INFORMATION ON SPECIMEN

(57)Abstract:
PROBLEM TO BE SOLVED: To provide a new method, in which the information on specimen is obtained with higher accuracy in a nondestructive state, by using a near- infrared spectrum.
SOLUTION: In the method which obtains the information on a specimen, (a) a process in which the specimen is irradiated with continuous wavelength light in the region of 400 to 2,500 nm or in a part of it and (b) a process, in which a peak in the obtained spectrum is decomposed to an element peak by a spectroscopic technique are contained. More specifically, the method discriminates a group to which an unknown specimen belongs, the method identifies the unknown specimen and monitors the aged deterioration of the specimen in real time. By this method, the information on the specimen can be obtained with higher accuracy, at a low cost, through the element peak of water molecules and in the nondestructive state by using a comparatively simple apparatus.



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decision of rejection]
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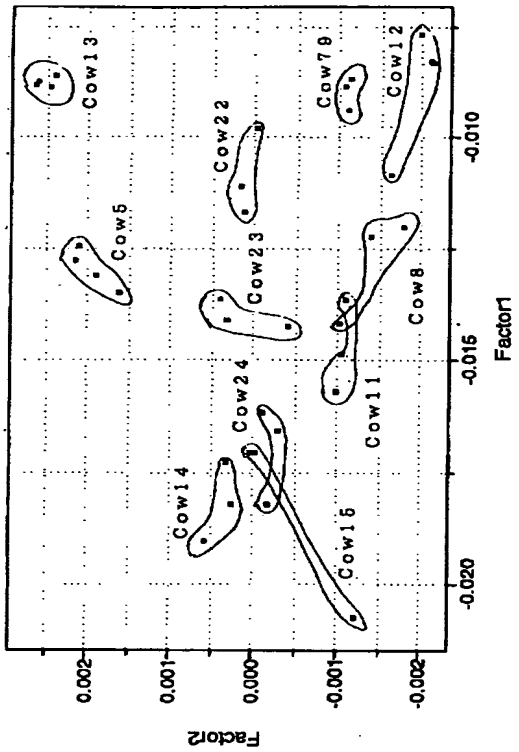
Drawing selection Representative drawing



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JAPANESE [JP,2002-005827,A]

CLAIMS DETAILED DESCRIPTION TECHNICAL FIELD PRIOR ART EFFECT OF THE INVENTION TECHNICAL PROBLEM MEANS EXAMPLE DESCRIPTION OF DRAWINGS DRAWINGS

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CLAIMS

[Claim(s)]
[Claim 1] (a) How to acquire the information on analyte which irradiates continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm, and includes in analyte the process which decomposes into an element peak the peak in the process which obtains the spectrum of analyte, and the spectrum (b) Obtained by the spectroscopy-technique.
[Claim 2] The approach according to claim 1 by which analyte is chosen from a natural product, artifacts, and those workpieces.
[Claim 3] The approach according to claim 1 by which analyte is chosen as a living body (except for Homo sapiens), agricultural products and its workpiece, a livestock product and its workpiece, and a list from marine products and its workpiece.
[Claim 4] The approach according to claim 1 the spectroscopy-technique is secondary differential processing.
[Claim 5] (a) Irradiate continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm at each analyte belonging to the specific group which consists of two or more analytes. Decompose into an element peak the process which obtains the spectrum of each analyte, and the peak in each spectrum (b) Obtained by the spectroscopy-technique, and multivariate analysis of the element peak of the water molecule in it is carried out. How to present the spectroscopy-technique of the exposure of the light of the above-mentioned process (a), and the above-mentioned process (b) with the process which creates the analytic model of the group, and the analyte of (c) strangeness, and include the process which distinguishes the group to which strange analyte belongs from the spectrum pattern of the element peak of the water molecule.
[Claim 6] The approach according to claim 5 by which analyte is chosen from a natural product, artifacts, and those workpieces.
[Claim 7] The approach according to claim 5 by which analyte is chosen as a living body (except for Homo sapiens), agricultural products and its workpiece, a livestock product and its workpiece, and a list from marine products and its workpiece.
[Claim 8] The approach according to claim 5 multivariate analysis is principal component analysis.
[Claim 9] The approach according to claim 5 the spectroscopy-technique is secondary differential processing.
[Claim 10] The approach according to claim 5 of being the approach of distinguishing the normal or the abnormalities of analyte.
[Claim 11] (a) Irradiate continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm at analyte. Decompose into an element peak the process which obtains the spectrum of analyte, and the peak in each spectrum (b) Obtained by the spectroscopy-technique, and multivariate analysis of the element peak of the water molecule in it is carried out. How to present the spectroscopy-technique of the exposure of the light of the above-mentioned process (a), and the above-mentioned process (b) with the process which creates the analytic model of analyte, and the analyte of (c) strangeness, and include the process which identifies strange analyte from the spectrum pattern of the element peak of the water molecule.
[Claim 12] The approach according to claim 11 by which analyte is chosen from a natural product, artifacts, and those workpieces.
[Claim 13] The approach according to claim 11 by which analyte is chosen as a living body

(except for Homo sapiens), agricultural products and its workpiece, a livestock product and its workpiece, and a list from marine products and its workpiece.
[Claim 14] The approach according to claim 11 multivariate analysis is principal component analysis.
[Claim 15] The approach according to claim 11 the spectroscopy-technique is secondary differential processing.
[Claim 16] (a) the process which decomposes into an element peak the process which irradiates continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm, and obtains two or more spectrums of analyte periodically to analyte, and the peak in each spectrum (b) obtained by the spectroscopy-technique, and (c) -- the approach of including the process which acts as the monitor of the aging in the analyte concerned on real time from the spectrum pattern of the element peak of those water molecules.
[Claim 17] The approach according to claim 16 by which analyte is chosen from a natural product, artifacts, and those workpieces.
[Claim 18] The approach according to claim 16 by which analyte is chosen as a living body (except for Homo sapiens), agricultural products and its workpiece, a livestock product and its workpiece, and a list from marine products and its workpiece.
[Claim 19] The approach according to claim 16 the spectroscopy-technique is secondary differential processing.

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DETAILED DESCRIPTION

[Detailed Description of the Invention]
[0001]
[Field of the Invention] This invention relates to the approach of acquiring the information on analyte that the visible-near infrared ray was used, the approach of specifically distinguishing the group to which strange analyte belongs, the method of identifying strange analyte, and the approach of acting as the monitor of the aging in analyte on real time.
[0002]
[Description of the Prior Art] In recent years, analysis using a near infrared ray is performed in various fields. For example, a near infrared ray is irradiated at analyte and it is used for carrying out quantitative analysis of the specific component.
[0003] Generally, the absorbancy index of a near infrared ray of the matter is very small, and since it is hard to receive dispersion, it has high permeability to a thick body. Therefore, analysis of analyte is possible in the state of un-destroying. Moreover, since a near infrared ray is the low electromagnetic wave of energy, it hardly damages analyte.
[0004] For analysis of the sugar content of fruits, such as the quantitative analysis of the specific component using an above-mentioned near infrared ray, for example, a melon, and a watermelon, the sugar content was computed from the data obtained from the peak to which it was limited in the near-infrared spectrum, and the calibration curve of the sugar content for which it asked beforehand. Such quantitative analysis is used in agriculture and the food field.
[0005] However, in the above analysis, only quantitative analysis of a specific component could be carried out and distinction (for example, distinction of the gun-ized mouse and a normal mouse) with the unusual analyte which caused qualitative analysis, for example, inflammation etc., and normal analyte, distinction between the analytes of a similar class (for example, distinction of the meat of the **** origin and the meat of the other pig origins), identification (for example, identification of each cow) of each analyte, etc. were not able to be performed. These analysis had the problem of expensive instrument for analysis being required like DNA analysis, or an analysis procedure being complicated, needing advanced skill, or long duration needing for analysis.
[0006]
[Problem(s) to be Solved by the Invention] The purpose of this invention is in the condition of having used the near-infrared spectrum and of not destroying, is a higher precision, and is to offer the new approach for acquiring the information on analyte.
[0007]
[Means for Solving the Problem] this invention person paid his attention to the hydrogen bond condition of the water molecule which exists in analyte, and other constituents. And when it decomposed into the element peak by the spectroscopy-technique and the peak in the visible-near-infrared spectrum of analyte was studied about the relation between the element peak of the water molecule in it, and the above-mentioned hydrogen bond condition, knowledge that the element peak of this water molecule shifts by the interaction (change of a hydrogen bond condition) of a water molecule and other constituents or an absorbance changes was acquired. And it turned out that it lets the element peak of this water molecule pass, and it becomes possible to acquire the information on analyte in a higher precision. It lets the element peak of the water molecule in such a visible-near-infrared spectrum of analyte pass, and the method of acquiring the information on analyte will not be performed without this invention person.

[0008] That is, this invention is as follows. (1) How to acquire the information on analyte which irradiates continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm, and includes the process which decomposes into an element peak the peak in the process which obtains the spectrum of analyte, and the spectrum (b) Obtained by the spectroscopy-technique in (a) analyte.
(2) The approach of the above-mentioned (1) publication that analyte is chosen from a natural product, artifacts, and those workpieces.
(3) The approach of the above-mentioned (1) publication that analyte is chosen as a living body (except for Homo sapiens), agricultural products and its workpiece, a livestock product and its workpiece, and a list from marine products and its workpiece.
(4) The approach of the above-mentioned (1) publication that the spectroscopy-technique is secondary differential processing.
(5) (a) Continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm is irradiated at each analyte belonging to the specific group which consists of two or more analytes. Decompose into an element peak the process which obtains the spectrum of each analyte, and the peak in each spectrum (b) Obtained by the spectroscopy-technique, and multivariate analysis of the element peak of the water molecule in it is carried out. How to present the spectroscopy-technique of the exposure of the light of the above-mentioned process (a), and the above-mentioned process (b) with the process which creates the analytic model of the group, and the analyte of (c) strangeness, and include the process which distinguishes the group to which strange analyte belongs from the spectrum pattern of the element peak of the water molecule.
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(7) The approach of the above-mentioned (5) publication that analyte is chosen as a living body (except for Homo sapiens), agricultural products and its workpiece, a livestock product and its workpiece, and a list from marine products and its workpiece.
(8) The approach of the above-mentioned (5) publication that multivariate analysis is principal component analysis.
(9) The approach of the above-mentioned (5) publication that the spectroscopy-technique is secondary differential processing.
(10) The approach of the above-mentioned (5) publication which is the approach of distinguishing the normal or the abnormalities of analyte.
(11) Irradiate continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm at (a) analyte. Decompose into an element peak the process which obtains the spectrum of analyte, and the peak in each spectrum (b) Obtained by the spectroscopy-technique, and multivariate analysis of the element peak of the water molecule in it is carried out. How to present the spectroscopy-technique of the exposure of the light of the above-mentioned process (a), and the above-mentioned process (b) with the process which creates the analytic model of analyte, and the analyte of (c) strangeness, and include the process which identifies strange analyte from the spectrum pattern of the element peak of the water molecule.
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(14) The approach of the above-mentioned (11) publication that multivariate analysis is principal component analysis.
(15) The approach of the above-mentioned (11) publication that the spectroscopy-technique is secondary differential processing.
(16) Irradiate continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm periodically at (a) analyte. (b) b [the process which obtains two or more spectrums of analyte, and] the peak in each obtained spectrum the process decomposed into an element peak by the spectroscopy-technique, and (c) -- the approach of including the process which acts as the monitor of the aging in the analyte concerned on real time from the spectrum pattern of the element peak of those water molecules.
(17) The approach of the above-mentioned (16) publication that analyte is chosen from a

natural product, artifacts, and those workpieces.
(18) The approach of the above-mentioned (16) publication that analyte is chosen as a living body (except for Homo sapiens), agricultural products and its workpiece, a livestock product and its workpiece, and a list from marine products and its workpiece.
(19) The approach of the above-mentioned (16) publication that the spectroscopy-technique is secondary differential processing.
[0009]
[Embodiment of the Invention] Hereafter, this invention is explained to a detail. In this invention, first, to analyte, continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm is irradiated, and the spectrum of analyte is obtained.
[0010] In this invention, "continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm" is the light to which the light to which wavelength was continuously changed over the whole range of the range of 400nm - 2500nm or some its range (for example, 600-1000nm) was said to, for example, it changed 1nm of wavelength at a time continuously from 600nm to 1000nm.
[0011] Especially as a near infrared ray spectrophotometer used by this invention, there is no limit and a well-known near infrared ray spectrophotometer can be used.
[0012] Subsequently, the peak in the obtained spectrum is decomposed into an element peak by the spectroscopy-technique. In this invention, as the spectroscopy-technique decomposed into an element peak, although secondary differential processing, the Fourier transform, web let conversion, the neural network method, etc. are illustrated, this invention is not limited to these but all also of the well-known spectroscopy-technique and the new spectroscopy-technique after this invention are contained in this invention, for example. Moreover, the spectroscopy-technique needed for analysis of analyte information chooses, and it is used.
[0013] In creating a model next, it carries out multivariate analysis of the element peak of the water molecule in the above-mentioned element peak. As multivariate analysis which can be used by this invention, although principal component analysis, factor analysis, cluster analysis, SIMCA (soft independent modeling of class analogy), etc. are illustrated, this invention is not limited to these but all also of well-known multivariate analysis and the new multivariate analysis after this invention are contained in this invention. Moreover, the multivariate analysis needed for analysis of analyte information chooses, and is used.
[0014] It is desirable to use SIMCA at the point which has a more realistic prediction function also in the above. SIMCA is the principal component analysis for every group, and strange analyte can distinguish to which class it belongs, or whether it belongs.
[0015] Specifically principal component analysis of the element peak of the water molecule of analyte is carried out for every group, information is mutually summarized in two or more principal components [**** /-less], and a principal component model is created for every group based on distribution of these principal component scores. And it distinguishes by SIMCA to which group strange analyte belongs, or whether it belongs.
[0016] It is thought that the physicochemical property of water is very specific, and this is based on the hydrogen bond condition of a water molecule. It is known that there are nine kinds of hydrogen bond conditions of a water molecule, and it is also known that they will be classified into five sorts. Moreover, it is also known that the peak of an about 970nm water molecule will be decomposed into the element peak of five sorts of water molecules from which a hydrogen bond condition differs.
[0017] In water, water molecules are carrying out hydrogen bond. If other components are added here, cutting will arise in the hydrogen bond between water molecules, or a hydrogen bond condition -- new hydrogen bond is formed between a water molecule and other components -- will change. When the most, analyte contains a lot of water, and contains other constituents other than water.
[0018] this invention person acquired the knowledge that the element peak of a water molecule shifted or reinforcement changed with the interactions (change of a hydrogen bond condition) of a water molecule and other components, as a result of decomposing the peak in a visible-near-infrared spectrum into an element peak by the spectroscopy-technique and studying wholeheartedly the relation between the element peak of the water molecule in it, and the hydrogen bond condition of a water molecule and other components.
[0019] About what added a lactose, NaCl, or albumin in water and water, respectively this

invention person irradiated the 600-1000nm near infrared ray, decomposed the peak in a spectrum into the element peak by the spectroscopy-technique, and did principal component analysis of the element peak of the water molecule in it. The 1st and 2nd principal component loading at that time is shown in drawing 1 -4. Moreover, the element peak of a water molecule shown by this loading is shown in Table 1. Here, obtain a spectrum by the above-mentioned approach, respectively about a 5.26g [/ml] lactose water solution, a 1.27g [/ml] NaCl water solution, and a 2.56g [/ml] albumin water solution, and two fold serial dilution of these solutions is carried out after that. It repeats so that it may say that a spectrum is obtained similarly, respectively, two fold serial dilution is carried out further, and a spectrum is obtained similarly, respectively. About the lactose water solution, the NaCl water solution, and the albumin water solution, the spectrum of 15 was obtained, respectively, these were decomposed into the element peak by the above-mentioned approach, and principal component analysis of the element peak of the water molecule in it was carried out.

[0020] in addition, the near-infrared spectrophotometer (the product made from Fantoc, FRUIT TESTER20, 1mm of cel length) was used for measurement of a near-infrared spectrum, and the 600-1000nm near infrared ray was irradiated at intervals of 1nm from 600nm up to 1000nm. In order to change the obtained spectrum T into an absorbance spectrum, log (1/T) was calculated, and subsequently smoothing processing was carried out. Subsequently, secondary differential processing of the peak in a spectrum was carried out, it decomposed into the element peak and principal component analysis of the element peak of the water molecule in it was carried out. Pirouette2.6 (GL Saiensu-Sha Co., Ltd. make) was used for these processings of a series of as data-processing software.

[0021]

[Table 1]

Water	Water(W)	Water(W)	Water(W)
	W + Lact	W + NaCl	W + Alb
618nm			
624		622	
628		630	
638			
		648	
652	656	654	654
662		664	
	676	676	
690	690	690	694
704		708	
716			
724			
	730	730	728
740		740	
746	744		
760	760	762	762
770			
782	780	780	778
794	796	798	796
810	810		
814		814	816
		828	
830	838		834
842		846	
858			
872			
874	878	876	876
886		890	
898			
914	908	910, 914	916
934	932	932	932
946			
	952	950	958
964	962	968	968
	974		
984		972	
	992		

[0022] Table 1 shows that the element peak of those water molecules has shifted to water in what added a lactose, NaCl, or albumin compared with the element peak of the water molecule in a water independent.

[0023] for example, -- typical -- water -- element peak 652nm of the water molecule which can be set independently, 724nm, 740nm, 782nm, 794nm, 842nm, 872nm, 934nm and 964nm be understood that it have shifted to 656nm, 730nm, 744nm, 780nm, 796nm, 838nm, 878nm, 932nm and 962nm, respectively in what added the lactose in water.

[0024] Moreover, element peak 624nm of a water molecule [in / typically / a water independent], 628nm, 652nm, 662nm, 704nm, 724nm, 760nm, 782nm, 794nm, 830nm, 842nm, 872nm, 886nm, 934nm, and 964nm In what added NaCl in water, respectively 622nm, 630nm, It turns out that it has shifted to 654nm, 664nm, 708nm, 730nm, 762nm, 780nm, 798nm, 828nm, 846nm, 876nm, 890nm, 932nm, and 968nm.

[0025] Furthermore, element peak 652nm of a water molecule [in / typically / a water independent], 690nm, 724nm, 760nm, 782nm, 794nm, 814nm, 830nm, 874nm, 934nm, and 964nm In what added albumin in water, it turns out that it has shifted to 654nm, 694nm, 728nm, 762nm, 778nm, 796nm, 816nm, 834nm, 876nm, 932nm, and 968nm, respectively.
[0026] Thus, if a hydrogen bond condition changes with addition (existence) of other components, the element peak of the water molecule in a spectrum will be shifted (or reinforcement changes). Other classes and amounts of a constituent (all components other than the water in analyte are said) other than the water which exists in analyte change with each analytes, and, therefore, the hydrogen bond condition of the water molecule in analyte and other constituents is peculiar to analyte. Therefore, the element peak of this water molecule that may change with the hydrogen bond conditions of the water in analyte and other constituents (reinforcement may change or it can shift) can be regarded as an element peak of the water molecule of a proper to analyte. It lets the element peak of the water molecule of such a proper pass, and it becomes possible to acquire the information on analyte simply in a higher precision.
[0027] An analytic model with a precision high concrete more can be created, it is a higher precision and the distinction of a group and the identification of strange analyte to which strange analyte belongs are attained from this analytic model. Moreover, it also becomes possible from the spectrum pattern of the element peak of a water molecule to act as the monitor of the aging of the information in analyte on real time.
[0028] As analyte in this invention, although there is especially no limit, it may need nondestructive analysis preferably and any of a natural product, artifacts, and those workpieces are sufficient as it.

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TECHNICAL FIELD

[Field of the Invention] This invention relates to the approach of acquiring the information on analyte that the visible-near infrared ray was used, the approach of specifically distinguishing the group to which strange analyte belongs, the method of identifying strange analyte, and the approach of acting as the monitor of the aging in analyte on real time.

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PRIOR ART

[Description of the Prior Art] In recent years, analysis using a near infrared ray is performed in various fields. For example, a near infrared ray is irradiated at analyte and it is used for carrying out quantitative analysis of the specific component.
[0003] Generally, the absorbancy index of a near infrared ray of the matter is very small, and since it is hard to receive dispersion, it has high permeability to a thick body. Therefore, analysis of analyte is possible in the state of un-destroying. Moreover, since a near infrared ray is the low electromagnetic wave of energy, it hardly damages analyte.
[0004] For analysis of the sugar content of fruits, such as the quantitative analysis of the specific component using an above-mentioned near infrared ray, for example, a melon, and a watermelon, the sugar content was computed from the data obtained from the peak to which it was limited in the near-infrared spectrum, and the calibration curve of the sugar content for which it asked beforehand. Such quantitative analysis is used in agriculture and the food field.
[0005] However, in the above analysis, only quantitative analysis of a specific component could be carried out and distinction (for example, distinction of the gun-ized mouse and a normal mouse) with the unusual analyte which caused qualitative analysis, for example, inflammation etc., and normal analyte, distinction between the analytes of a similar class (for example, distinction of the meat of the **** origin and the meat of the other pig origins), identification (for example, identification of each cow) of each analyte, etc. were not able to be performed. These analysis had the problem of expensive instrument for analysis being required like DNA analysis, or an analysis procedure being complicated, needing advanced skill, or long duration needing for analysis.

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EFFECT OF THE INVENTION

[Effect of the Invention] According to this invention, the peak in a visible-near-infrared spectrum is decomposed into an element peak by the spectroscopy-technique, and it lets the element peak of the water molecule in it pass, and in the state of un-destroying, using comparatively easy equipment, quickness can be acquired in a higher precision and the information on analyte can be acquired by low cost.

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TECHNICAL PROBLEM

[Problem(s) to be Solved by the Invention] The purpose of this invention is in the condition of having used the near-infrared spectrum and of not destroying, is a higher precision, and is to offer the new approach for acquiring the information on analyte.

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MEANS

[Means for Solving the Problem] this invention person paid his attention to the hydrogen bond condition of the water molecule which exists in analyte, and other constituents. And when it decomposed into the element peak by the spectroscopy-technique and the peak in the visible-near-infrared spectrum of analyte was studied about the relation between the element peak of the water molecule in it, and the above-mentioned hydrogen bond condition, knowledge that the element peak of this water molecule shifts by the interaction (change of a hydrogen bond condition) of a water molecule and other constituents or an absorbance changes was acquired. And it turned out that it lets the element peak of this water molecule pass, and it becomes possible to acquire the information on analyte in a higher precision. It lets the element peak of the water molecule in such a visible-near-infrared spectrum of analyte pass, and the method of acquiring the information on analyte will not be performed without this invention person.
[0008] That is, this invention is as follows. (1) How to acquire the information on analyte which irradiates continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm, and includes the process which decomposes into an element peak the peak in the process which obtains the spectrum of analyte, and the spectrum (b) Obtained by the spectroscopy-technique in (a) analyte.
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(13) The approach of the above-mentioned (11) publication that analyte is chosen as a living body (except for Homo sapiens), agricultural products and its workpiece, a livestock product and its workpiece, and a list from marine products and its workpiece.
(14) The approach of the above-mentioned (11) publication that multivariate analysis is principal component analysis.
(15) The approach of the above-mentioned (11) publication that the spectroscopy-technique is secondary differential processing.
(16) Irradiate continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm periodically at (a) analyte. (b) b [the process which obtains two or more spectrums of analyte, and] the peak in each obtained spectrum the process decomposed into an element peak by the spectroscopy-technique, and (c) -- the approach of including the process which acts as the monitor of the aging in the analyte concerned on real time from the spectrum pattern of the element peak of those water molecules.
(17) The approach of the above-mentioned (16) publication that analyte is chosen from a natural product, artifacts, and those workpieces.
(18) The approach of the above-mentioned (16) publication that analyte is chosen as a living body (except for Homo sapiens), agricultural products and its workpiece, a livestock product and its workpiece, and a list from marine products and its workpiece.
(19) The approach of the above-mentioned (16) publication that the spectroscopy-technique is secondary differential processing.
[0009]
[Embodiment of the Invention] Hereafter, this invention is explained to a detail. In this invention, first, to analyte, continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm is irradiated, and the spectrum of analyte is obtained.
[0010] In this invention, "continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm" is the light to which the light to which wavelength was continuously changed over the whole range of the range of 400nm - 2500nm or some its range (for example, 600-1000nm) was said to, for example, it changed 1nm of wavelength at a time continuously from 600nm to 1000nm.
[0011] Especially as a near infrared ray spectrophotometer used by this invention, there is no limit and a well-known near infrared ray spectrophotometer can be used.
[0012] Subsequently, the peak in the obtained spectrum is decomposed into an element peak by the spectroscopy-technique. In this invention, as the spectroscopy-technique decomposed into an element peak, although secondary differential processing, the Fourier transform, web let conversion, the neural network method, etc. are illustrated, this invention is not limited to these but all also of the well-known spectroscopy-technique and the new spectroscopy-technique after this invention are contained in this invention, for example. Moreover, the spectroscopy-technique needed for analysis of analyte information chooses, and it is used.
[0013] In creating a model next, it carries out multivariate analysis of the element peak of the water molecule in the above-mentioned element peak. As multivariate analysis which can be used by this invention, although principal component analysis, factor analysis, cluster analysis, SIMCA (soft independent modeling of class analogy), etc. are illustrated, this invention is not limited to these but all also of well-known multivariate analysis and the new multivariate analysis after this invention are contained in this invention. Moreover, the multivariate analysis needed for analysis of analyte information chooses, and is used.
[0014] It is desirable to use SIMCA at the point which has a more realistic prediction function also in the above. SIMCA is the principal component analysis for every group, and strange

analyte can distinguish to which class it belongs, or whether it belongs.
[0015] Specifically principal component analysis of the element peak of the water molecule of analyte is carried out for every group, information is mutually summarized in two or more principal components [**** /-less], and a principal component model is created for every group based on distribution of these principal component scores. And it distinguishes by SIMCA to which group strange analyte belongs, or whether it belongs.
[0016] It is thought that the physicochemical property of water is very specific, and this is based on the hydrogen bond condition of a water molecule. It is known that there are nine kinds of hydrogen bond conditions of a water molecule, and it is also known that they will be classified into five sorts. Moreover, it is also known that the peak of an about 970nm water molecule will be decomposed into the element peak of five sorts of water molecules from which a hydrogen bond condition differs.
[0017] In water, water molecules are carrying out hydrogen bond. If other components are added here, cutting will arise in the hydrogen bond between water molecules, or a hydrogen bond condition -- new hydrogen bond is formed between a water molecule and other components -- will change. When the most, analyte contains a lot of water, and contains other constituents other than water.
[0018] this invention person acquired the knowledge that the element peak of a water molecule shifted or reinforcement changed with the interactions (change of a hydrogen bond condition) of a water molecule and other components, as a result of decomposing the peak in a visible-near-infrared spectrum into an element peak by the spectroscopy-technique and studying wholeheartedly the relation between the element peak of the water molecule in it, and the hydrogen bond condition of a water molecule and other components.
[0019] About what added a lactose, NaCl, or albumin in water and water, respectively this invention person irradiated the 600-1000nm near infrared ray, decomposed the peak in a spectrum into the element peak by the spectroscopy-technique, and did principal component analysis of the element peak of the water molecule in it. The 1st and 2nd principal component loading at that time is shown in drawing 1 -4. Moreover, the element peak of a water molecule shown by this loading is shown in Table 1. Here, obtain a spectrum by the above-mentioned approach, respectively about a 5.26g [/ml] lactose water solution, a 1.27g [/ml] NaCl water solution, and a 2.56g [/ml] albumin water solution, and two fold serial dilution of these solutions is carried out after that. It repeats so that it may say that a spectrum is obtained similarly, respectively, two fold serial dilution is carried out further, and a spectrum is obtained similarly, respectively. About the lactose water solution, the NaCl water solution, and the albumin water solution, the spectrum of 15 was obtained, respectively, these were decomposed into the element peak by the above-mentioned approach, and principal component analysis of the element peak of the water molecule in it was carried out.
[0020] in addition, the near-infrared spectrophotometer (the product made from Fantoc, FRUIT TESTER20, 1mm of cel length) was used for measurement of a near-infrared spectrum, and the 600-1000nm near infrared ray was irradiated at intervals of 1nm from 600nm up to 1000nm. In order to change the obtained spectrum T into an absorbance spectrum, log (1/T) was calculated, and subsequently smoothing processing was carried out. Subsequently, secondary differential processing of the peak in a spectrum was carried out, it decomposed into the element peak and principal component analysis of the element peak of the water molecule in it was carried out. Pirouette2.6 (GL Saiensu-Sha Co., Ltd. make) was used for these processings of a series of as data-processing software.
[0021]
[Table 1]

Water	Water(W) W + Lact	Water(W) W + NaCl	Water(W) W + Alb
618nm			
624		622	
628		630	
638			
		646	
652	656	654	654
662		664	
	676	676	
690	690	690	694
704		708	
716			
724			
	730	730	728
740		740	
746	744		
760	760	762	762
770			
782	780	780	778
794	796	798	796
810	810		
814		814	816
		828	
830	838		834
842		846	
858			
872			
874	878	876	876
886		890	
898			
914	908	910, 914	916
934	932	932	932
946			
	952	950	958
964	962	968	968
	974		
984		972	
	992		

[0022] Table 1 shows that the element peak of those water molecules has shifted to water in what added a lactose, NaCl, or albumin compared with the element peak of the water molecule in a water independent.

[0023] for example, -- typical -- water -- element peak 652nm of the water molecule which can be set independently, 724nm, 740nm, 782nm, 794nm, 842nm, 872nm, 934nm and 964nm be understood that it have shifted to 656nm, 730nm, 744nm, 780nm, 796nm, 838nm, 878nm, 932nm and 962nm, respectively in what added the lactose in water.

[0024] Moreover, element peak 624nm of a water molecule [in / typically / a water independent], 628nm, 652nm, 662nm, 704nm, 724nm, 760nm, 782nm, 794nm, 830nm, 842nm, 872nm, 886nm, 934nm, and 964nm In what added NaCl in water, respectively 622nm, 630nm, It turns out that it has shifted to 654nm, 664nm, 708nm, 730nm, 762nm, 780nm, 798nm, 828nm, 846nm, 876nm, 890nm, 932nm, and 968nm.

[0025] Furthermore, element peak 652nm of a water molecule [in / typically / a water independent], 690nm, 724nm, 760nm, 782nm, 794nm, 814nm, 830nm, 874nm, 934nm, and 964nm In what added albumin in water, it turns out that it has shifted to 654nm, 694nm, 728nm, 762nm, 778nm, 796nm, 816nm, 834nm, 876nm, 932nm, and 968nm, respectively.
[0026] Thus, if a hydrogen bond condition changes with addition (existence) of other components, the element peak of the water molecule in a spectrum will be shifted (or reinforcement changes). Other classes and amounts of a constituent (all components other than the water in analyte are said) other than the water which exists in analyte change with each analytes, and, therefore, the hydrogen bond condition of the water molecule in analyte and other constituents is peculiar to analyte. Therefore, the element peak of this water molecule that may change with the hydrogen bond conditions of the water in analyte and other constituents (reinforcement may change or it can shift) can be regarded as an element peak of the water molecule of a proper to analyte. It lets the element peak of the water molecule of such a proper pass, and it becomes possible to acquire the information on analyte simply in a higher precision.
[0027] An analytic model with a precision high concrete more can be created, it is a higher precision and the distinction of a group and the identification of strange analyte to which strange analyte belongs are attained from this analytic model. Moreover, it also becomes possible from the spectrum pattern of the element peak of a water molecule to act as the monitor of the aging of the information in analyte on real time.
[0028] As analyte in this invention, although there is especially no limit, it may need nondestructive analysis preferably and any of a natural product, artifacts, and those workpieces are sufficient as it. Specifically, a living body, agricultural products (mammalians, such as a cow except Homo sapiens and a mouse, fishes, vegetation, etc.), such as cereals, vegetables, legumes, and seeds, or those workpieces, livestock products (cow's milk, meat, etc.) or those workpieces, marine products or those workpieces, soil, wood, drugs, etc. are mentioned.
[0029] As qualitative information in this invention, the following are mentioned, for example.
1. Distinguish to which group analyte belongs. For example, the normal and the abnormalities of analyte are distinguished. Specifically, a living body (except for Homo sapiens) distinguishes [abnormalities (for example, illnesses, such as a gun and inflammation) or] whether it is normal. Moreover, the place of production of analyte is distinguished. Specifically, places of production, such as perfume, an soybean, and wheat, are distinguished. furthermore, a relative -- the analyte between seeds is distinguished. Specifically, the meat of the **** origin or the meat of the other pig origins is distinguished. Furthermore, the grade of analyte is distinguished. Specifically, a grade is distinguished with the freshness of a marine product and agricultural products. Furthermore, it distinguishes whether it has the quality of level with analyte. Specifically, quality is distinguished by the degree of the heat denaturation which protein received at the time of food processing.
[0030] The concrete distinction approach is performed by the following procedure. First, to each analyte belonging to the specific group (for example, a normal and abnormality exception, place-of-production exception, classification, and grade exception, according to quality) which consists of two or more analytes, continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm is irradiated, and the spectrum of each analyte is obtained.
[0031] Subsequently, the peak in each obtained spectrum is decomposed into an element peak by the spectroscopy-technique (for example, secondary differential processing), and multivariate analysis (for example, principal component analysis) of the element peak of the water molecule in it is carried out, and the analytic model (for example, principal component model) of those groups is created.
[0032] Subsequently, the exposure of the same light as the above and the spectroscopy-technique are presented with strange analyte, and the group to which strange analyte belongs is distinguished from the spectrum pattern of the element peak of the water molecule. Specifically, it distinguishes from the distance of the spectrum pattern of the element peak of the water molecule, and the model of each group by SIMCA. Thus, for example, a place of production, a kind, a grade, quality, an individual, and normal and abnormalities are discriminable.
[0033] 2. Identify an individual (each analyte). For example, each living body (for example, cow) is identified. By this approach, it can manage using the information on a proper to each living body like the fingerprint in human being, without attaching a tag to each cow one by one. Moreover, the origin of each analyte can also be identified. For example, if the livestock

products of each beef, cow's milk, etc. are identified, it can be identified whether it is what originates in which cow, respectively.

[0034] The concrete identification approach is performed by the following procedure. First, to analyte, continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm is irradiated, and the spectrum of analyte is obtained.

[0035] Subsequently, the peak in the obtained spectrum is decomposed into an element peak by the spectroscopy-technique (for example, secondary differential processing). When the exposure to analyte is 2 times or more, multivariate analysis (for example, principal component analysis) of the element peak of the water molecule in it is carried out, and the analytic model (for example, principal component model) of analyte is created. When the exposure to analyte is only 1 time, let the spectrum pattern of the element peak of a water molecule be the spectrum pattern of a proper at analyte.

[0036] Subsequently, the exposure of the same light as the above and the spectroscopy-technique are presented with strange analyte, and strange analyte is identified from the spectrum pattern of the element peak of the water molecule. Specifically, it identifies by SIMCA from the distance of the spectrum pattern of the element peak of the water molecule, and the model of analyte. Or it is identified the spectrum pattern of the element peak of the water molecule by comparing the spectrum pattern of a proper with the analyte obtained beforehand.

[0037] 3. Act as the monitor of the aging of analyte on real time. The concrete monitor approach is performed by the following procedure. First, to analyte, periodically, continuous wave Nagamitsu of some [the] fields from 400nm to 2500nm is irradiated, and the spectrum of analyte is obtained.

[0038] Subsequently, the peak in each obtained spectrum is decomposed into an element peak by the spectroscopy-technique (for example, secondary differential processing). And it acts as the monitor of the aging in the analyte concerned on real time from the spectrum pattern of the element peak of those water molecules. Each spectrum pattern is compared and, specifically, it judges whether it is that aging arose (change of peak intensity, existence of a peak, etc.) at which element peak of a water molecule. Here, aging in one element peak may be seen and aging in two or more element peaks may be seen. Moreover, if multivariate analysis (for example, principal component analysis) of the element peak of the water molecule of all the above-mentioned spectrums is carried out, it can also know at which element peak aging has arisen (from for example, principal component loading). It can also predict what kind of aging has arisen from aging of the element peak of such a water molecule concretely in analyte.

[Translation done.]

* NOTICES *

1.This document has been translated by computer. So the translation may not reflect the original precisely.
2.**** shows the word which can not be translated.
3.In the drawings, any words are not translated.

EXAMPLE

[Example] Although an example is given and this invention is explained concretely hereafter, this invention is not limited to these examples.
[0040] the Example 1:distinction <use animal> mouse (CDF1 and a male mouse --) of the normal of a mouse, or abnormalities (gun-izing) The feed (benzpyrene dose: 0.5 mg/kg/day) which added the benzpyrene which is the cancerating substance, and additive-free feed are given to acquisition and 7 weeks old from Japan SLC, respectively. It bred for six months under conditions of the temperature of 25**2 degrees C, and 60**3% of humidity, the abnormality mouse group (a benzpyrene administration group, gun-ized mouse group) and the normal mouse group (benzpyrene group non-prescribing a medicine for the patient) were obtained, and these were offered as a sample. Each group of a normal group and an abnormality group (gun-izing) was made into seven animals.
[0041] the near-infrared spectrophotometer (the product made from Fantoc, FRUIT TESTER20) was used for measurement of a <measurement of spectrum> visible-near-infrared spectrum, and the 600-1000nm near infrared ray was irradiated about each mouse of a normal group and an abnormality group at the whole mouse at intervals of 1nm from 600nm up to 1000nm. In order to change each obtained spectrum T into an absorbance spectrum, log (1/T) was calculated and smoothing processing was carried out. Pirouette2.6 (GL Saiensu-Sha Co., Ltd. make) was used for these processings as data-processing software.
[0042] After performing <discernment of creation [of a principal component model], and abnormalities of mouse> smoothing processing, secondary differential processing decomposed the peak in each obtained spectrum into the element peak. Subsequently, principal component analysis of the element peak of the water molecule in it was carried out, and the principal component model of each group was created based on distribution of the extracted principal component score. The distribution (only the 1-3rd principal components) based on the principal component score of each group is shown in drawing 5 . Drawing 5 shows that the normal group and the abnormality group form one group, respectively. Moreover, the distance (distance between classes) of each group calculated by SIMCA is shown in Table 2. Table 2 shows that the distance between a normal group and an abnormality group is 1.1568. In addition, Pirouette2.6 (GL Saiensu-Sha Co., Ltd. make) was used for conversion of an absorbance spectrum, secondary differential processing, principal component analysis, and SIMCA as data-processing software.
[0043]
[Table 2]

		正常マウス群	異常マウス群
1	正常マウス群	0.0000	1.1568
2	異常マウス群	1.1568	0.0000

[0044] About the mouse which was not offered as a sample of the above-mentioned mice, near infrared ray exposure and secondary differential processing were performed by the same approach as the above, and it distinguished to which group it belongs, or whether it would belong by SIMCA from the distance of the spectrum pattern of the element peak of the water molecule, and the model of each group. It was able to distinguish by 90% or more of probability.

[0045]

* NOTICES *

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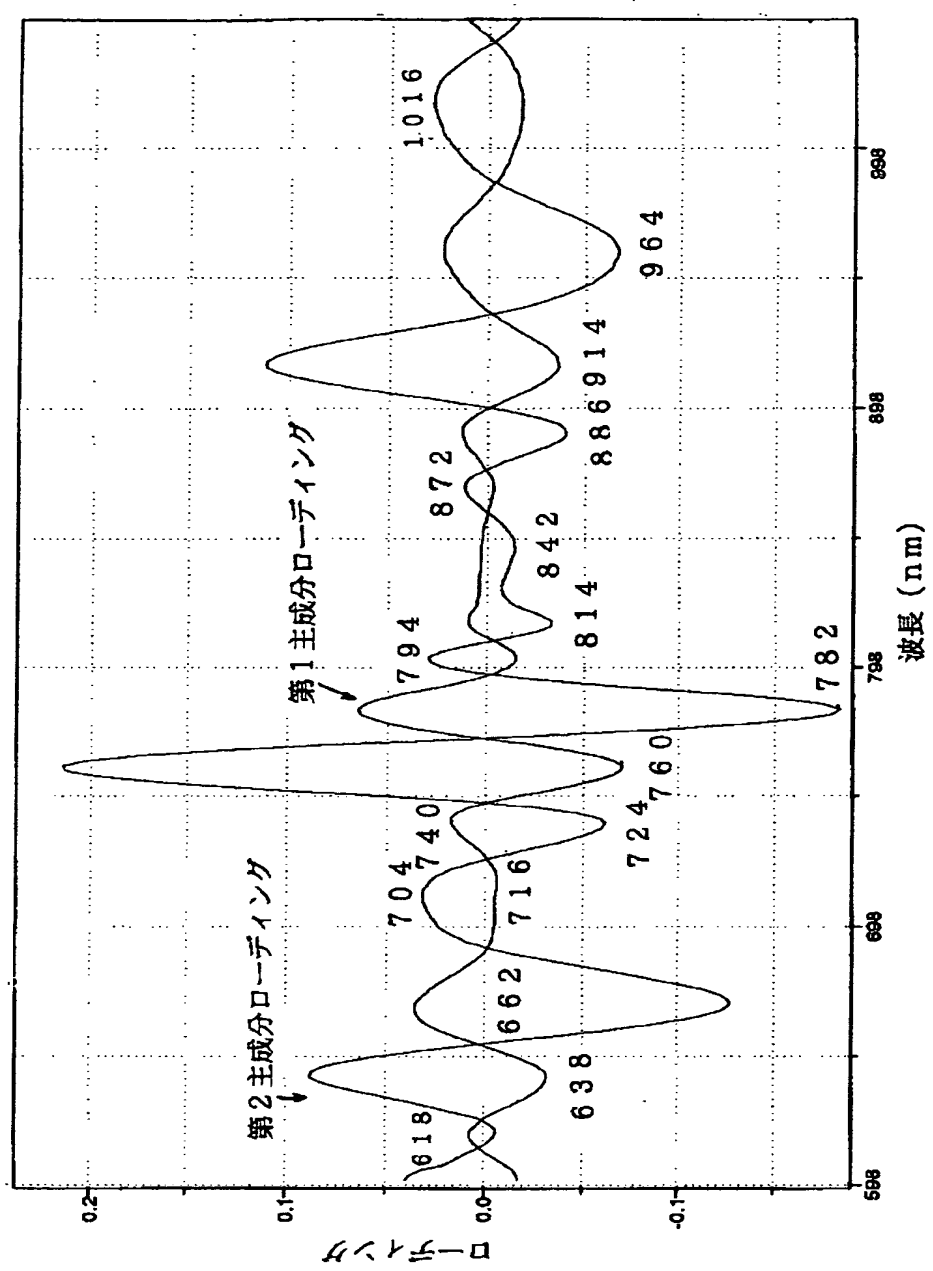
2.**** shows the word which can not be translated.
3.In the drawings, any words are not translated.

DESCRIPTION OF DRAWINGS

[Brief Description of the Drawings]
[Drawing 1] It is drawing showing loading of the 1st and 2nd principal components when carrying out principal component analysis of the element peak of the spectrum of water.
[Drawing 2] Although the lactose was added in water, it is drawing showing loading of the 1st and 2nd principal components when carrying out principal component analysis of the element peak of a spectrum.
[Drawing 3] Although NaCl was added in water, it is drawing showing loading of the 1st and 2nd principal components when carrying out principal component analysis of the element peak of a spectrum.
[Drawing 4] Although albumin was added in water, it is drawing showing loading of the 1st and 2nd principal components when carrying out principal component analysis of the element peak of a spectrum.
[Drawing 5] It is drawing showing the distribution based on the principal component score when carrying out principal component analysis of the element peak of the spectrum of a normal mouse group and an abnormality mouse group.
[Drawing 6] It is drawing showing the distribution based on the principal component score when carrying out principal component analysis of the element peak of the spectrum of the cow's milk with which the origins differ.
[Drawing 7] It is drawing showing the distribution based on the principal component score when carrying out principal component analysis of the element peak of the spectrum of each cow.
[Drawing 8] It is drawing in which carrying out secondary differential processing of the spectrum of the udder of a cow, and showing aging of the absorbance in element peak 840nm of the water molecule in it.

[Translation done.]

Drawing selection drawing 1



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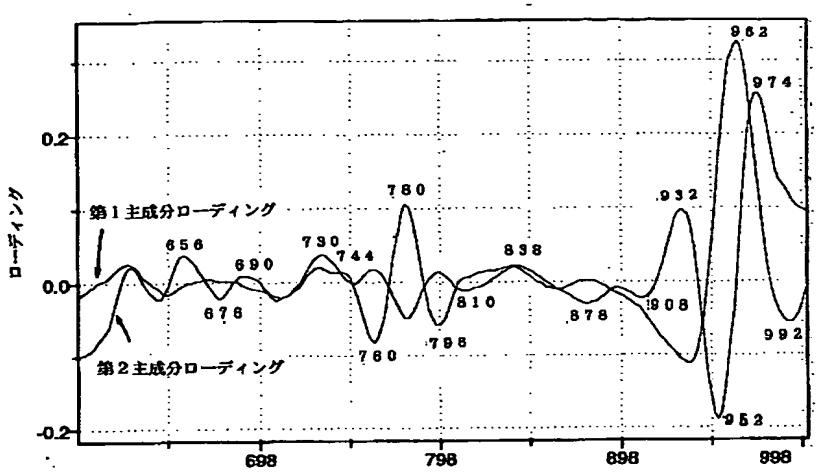

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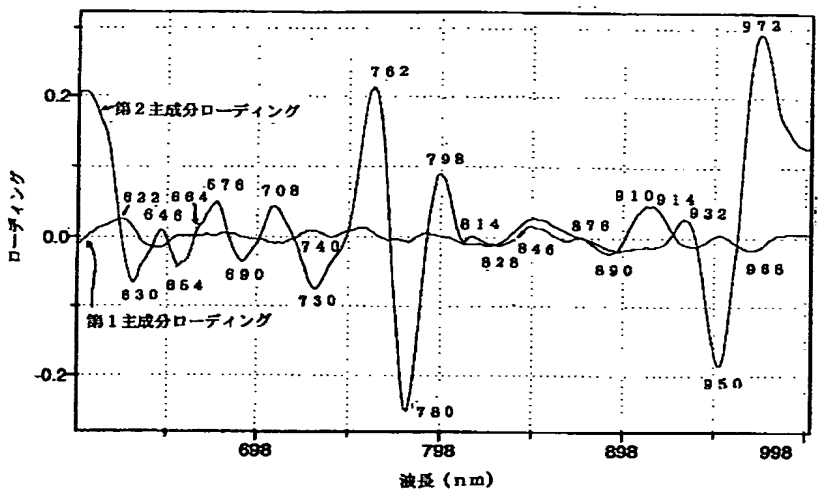

[Translation done.]

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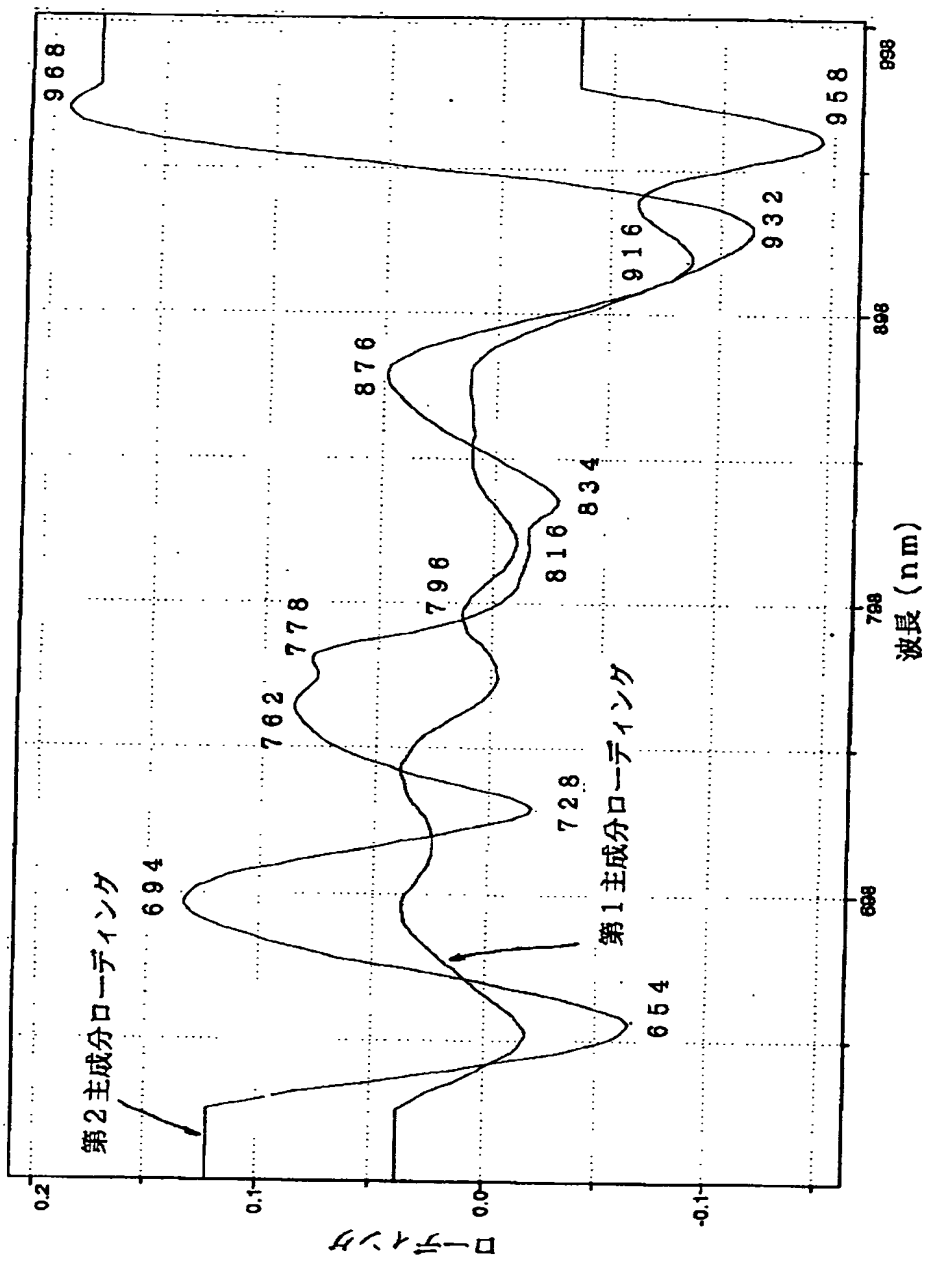

[Translation done.]

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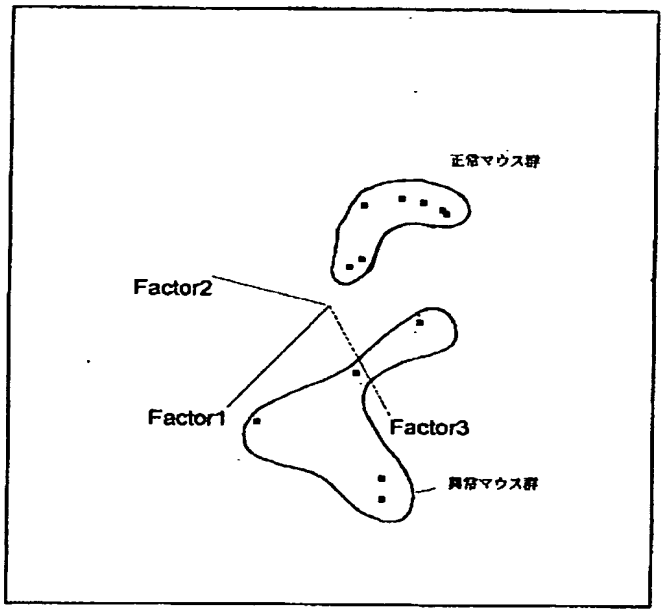
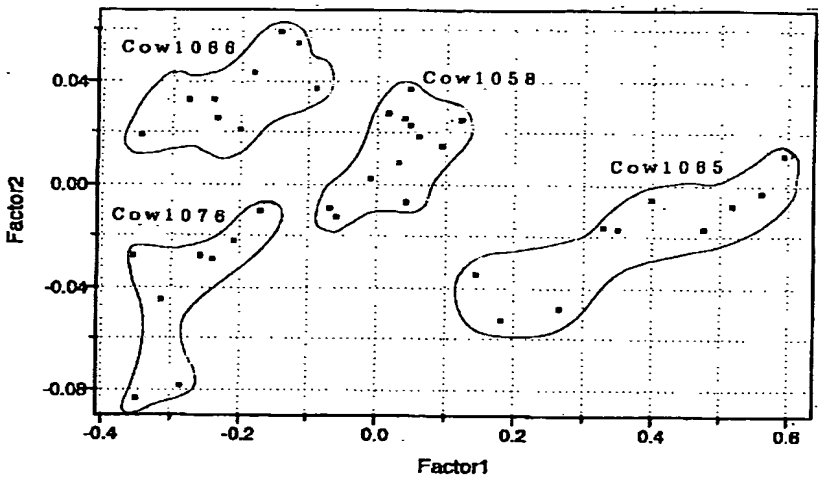


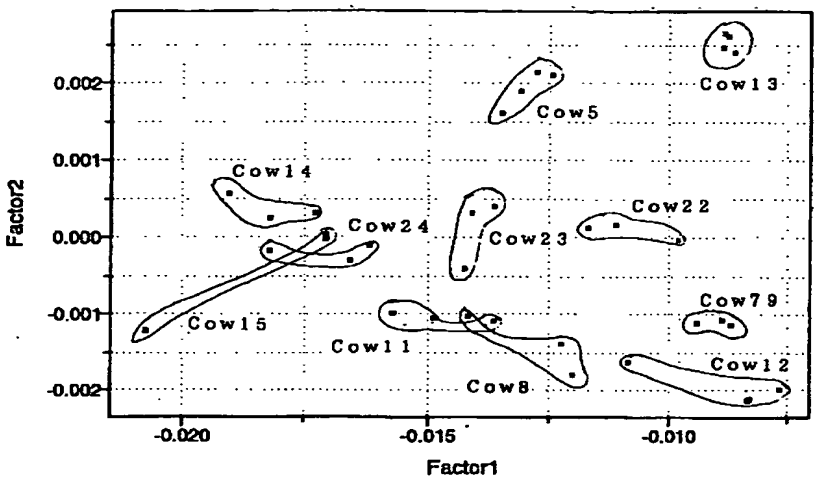
[Translation done.]

Drawing selection drawing 6



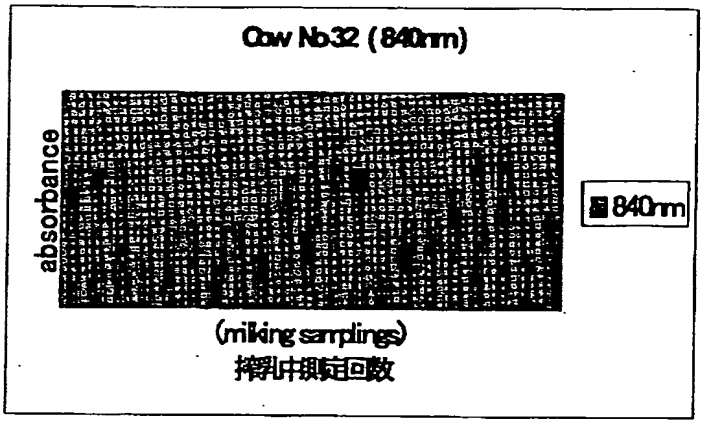
[Translation done.]

Drawing selection drawing 7



[Translation done.]

Drawing selection drawing 8



[Translation done.]

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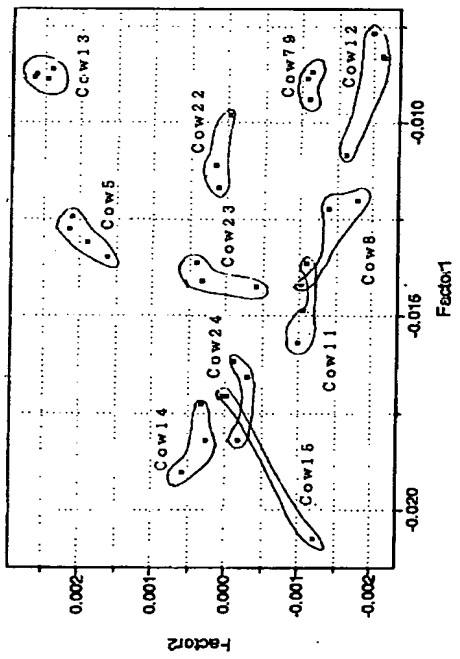
最終頁に続く

(54)【発明の名称】　被検体の情報を得る方法

(57)【要約】
【課題】　近赤外スペクトルを用いた、非破壊状態で、より高い精度で、被検体の情報を得るための新規な方法を提供する。
【解決手段】　（ａ）被検体に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、被検体のスペクトルを得る工程、および、（ｂ）得られたスペクトル中のピークを、分光学的手法により要素ピークに分解する工程、を含む、被検体の情報を得る方法。具体的には、未知の被検体が属する群を判別する方法、未知の被検体を同定する方法、および被検体の経時変化をリアルタイムでモニターする方法である。当該方法によれば、水分子の要素ピークを通して、非破壊状態で、比較的簡単な装置を用いて、より高い精度で迅速、低コストで、被検体の情報を得ることができる。



【特許請求の範囲】
【請求項１】　（ａ）被検体に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、被検体のスペクトルを得る工程、および、（ｂ）得られたスペクトル中のピークを、分光学的手法により要素ピークに分解する工程、を含む、被検体の情報を得る方法。
【請求項２】　被検体が、天然物、人工物およびそれらの加工品から選ばれる、請求項１記載の方法。
【請求項３】　被検体が、生体（ヒトを除く）、農産物およびその加工品、畜産物およびその加工品、並びに海産物およびその加工品から選ばれる、請求項１記載の方法。
【請求項４】　分光学的手法が２次微分処理である、請求項１記載の方法。
【請求項５】　（ａ）複数の被検体からなる特定の群に属する各被検体に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、各被検体のスペクトルを得る工程、（ｂ）得られた各スペクトル中のピークを、分光学的手法により要素ピークに分解し、その中の水分子の要素ピークを多変量解析して、その群の解析モデルを作成する工程、および、（ｃ）未知の被検体を、上記工程（ａ）の光の照射および上記工程（ｂ）の分光学的手法に供して、その水分子の要素ピークのスペクトルパターンから、未知の被検体の属する群を判別する工程、を含む、方法。
【請求項６】　被検体が、天然物、人工物およびそれらの加工品から選ばれる、請求項５記載の方法。
【請求項７】　被検体が、生体（ヒトを除く）、農産物およびその加工品、畜産物およびその加工品、並びに海産物およびその加工品から選ばれる、請求項５記載の方法。
【請求項８】　多変量解析が主成分分析である、請求項５記載の方法。
【請求項９】　分光学的手法が２次微分処理である、請求項５記載の方法。
【請求項１０】　被検体の正常または異常を判別する方法である、請求項５記載の方法。
【請求項１１】　（ａ）被検体に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、被検体のスペクトルを得る工程、（ｂ）得られた各スペクトル中のピークを、分光学的手法により要素ピークに分解し、その中の水分子の要素ピークを多変量解析して、被検体の解析モデルを作成する工程、および、（ｃ）未知の被検体を、上記工程（ａ）の光の照射および上記工程（ｂ）の分光学的手法に供して、その水分子の要素ピークのスペクトルパターンから、未知の被検体を同定する工程、を含む、方法。
【請求項１２】　被検体が、天然物、人工物およびそれらの加工品から選ばれる、請求項１１記載の方法。
【請求項１３】　被検体が、生体（ヒトを除く）、農産物およびその加工品、畜産物およびその加工品、並びに海産物およびその加工品から選ばれる、請求項１１記載の方法。
【請求項１４】　多変量解析が主成分分析である、請求項１１記載の方法。
【請求項１５】　分光学的手法が２次微分処理である、請求項１１記載の方法。
【請求項１６】　（ａ）被検体に、定期的に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、被検体の複数のスペクトルを得る工程、（ｂ）得られた各スペクトル中のピークを、分光学的手法により要素ピークに分解する工程、および、
（ｃ）それらの水分子の要素ピークのスペクトルパターンから、当該被検体における経時変化をリアルタイムでモニターする工程、を含む、方法。
【請求項１７】　被検体が、天然物、人工物およびそれらの加工品から選ばれる、請求項１６記載の方法。
【請求項１８】　被検体が、生体（ヒトを除く）、農産物およびその加工品、畜産物およびその加工品、並びに海産物およびその加工品から選ばれる、請求項１６記載の方法。
【請求項１９】　分光学的手法が２次微分処理である、請求項１６記載の方法。
【発明の詳細な説明】
【０００１】
【発明の属する技術分野】本発明は、可視－近赤外線を用いた被検体の情報を得る方法、具体的には、未知の被検体が属する群を判別する方法、未知の被検体を同定する方法、および被検体における経時変化をリアルタイムでモニターする方法に関する。
【０００２】
【従来の技術】近年、種々の分野で近赤外線を用いた分析が行われている。例えば、近赤外線を被検体に照射し、特定成分を定量分析することに用いられている。
【０００３】一般に、近赤外線は、物質の吸光係数が非常に小さく、散乱を受けにくいので、分厚い物体に対し高い透過性を有する。従って、非破壊状態で被検体の分析が可能である。また、近赤外線は、エネルギーの低い電磁波であるので、被検体を殆ど損傷することがない。
【０００４】上述の近赤外線を用いた特定成分の定量分析、例えば、メロン、スイカなどの果実類の糖度の分析には、近赤外スペクトル中の限定されたピークから得られたデータと、予め求めた糖度の検量線より、糖度を算出していた。このような定量分析は、農業、食品分野で利用されている。
【０００５】しかし、上記のような分析では特定成分の定量分析しか行えず、定性分析、例えば、炎症等を起こした異常な被検体と正常な被検体との判別（例えば、ガン化したマウスと正常なマウスの判別）、類似した種類

の被検体間の判別（例えば、黒豚由来の肉とその他の豚由来の肉の判別）、個々の被検体の同定（例えば、個々の牛の同定）等を行うことができなかった。これらの分析は、ＤＮＡ分析のように高価な分析機器が必要であったり、分析手順が煩雑であったり、高度の熟練を必要としたり、分析に長時間必要としたりする等の問題があった。

【０００６】

【発明が解決しようとする課題】本発明の目的は、近赤外スペクトルを用いた、非破壊状態で、より高い精度で、被検体の情報を得るための新規な方法を提供することにある。

【０００７】

【課題を解決するための手段】本発明者は、被検体中に存在する水分子と他の構成成分との水素結合状態に着目した。そして、被検体の可視－近赤外スペクトル中のピークを、分光学的手法により要素ピークに分解し、その中の水分子の要素ピークと、上記の水素結合状態との関係について研究したところ、この水分子の要素ピークが、水分子と他の構成成分との相互作用（水素結合状態の変化）によって、シフトしたり吸光度が変化したりするとの知見を得た。そして、この水分子の要素ピークを通して、より高い精度で、被検体の情報を得ることが可能となることがわかった。このような、被検体の可視－近赤外スペクトル中の水分子の要素ピークを通して、被検体の情報を得るという方法は、本発明者により初めて行われたものである。

【０００８】即ち、本発明は、以下のとおりである

(1) （ａ）被検体に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、被検体のスペクトルを得る工程、および、（ｂ）得られたスペクトル中のピークを、分光学的手法により要素ピークに分解する工程、を含む、被検体の情報を得る方法。

(2) 被検体が、天然物、人工物およびそれらの加工品から選ばれる、上記(1)記載の方法。

(3) 被検体が、生体（ヒトを除く）、農産物およびその加工品、畜産物およびその加工品、並びに海産物およびその加工品から選ばれる、上記(1)記載の方法。

(4) 分光学的手法が２次微分処理である、上記(1)記載の方法。

(5) （ａ）複数の被検体からなる特定の群に属する各被検体に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、各被検体のスペクトルを得る工程、（ｂ）得られた各スペクトル中のピークを、分光学的手法により要素ピークに分解し、その中の水分子の要素ピークを多変量解析して、その群の解析モデルを作成する工程、および、（ｃ）未知の被検体を、上記工程（ａ）の光の照射および上記工程（ｂ）の分光学的手法に供して、その水分子の要素ピークのスペクトルパターンから、未知の被検体の属する群を判別する工程、を含む、方法。

(6) 被検体が、天然物、人工物およびそれらの加工品から選ばれる、上記(5)記載の方法。

(7) 被検体が、生体（ヒトを除く）、農産物およびその加工品、畜産物およびその加工品、並びに海産物およびその加工品から選ばれる、上記(5)記載の方法。

(8) 多変量解析が主成分分析である、上記(5)記載の方法。

(9) 分光学的手法が２次微分処理である、上記(5)記載の方法。

(10) 被検体の正常または異常を判別する方法である、上記(5)記載の方法。

(11) （ａ）被検体に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、被検体のスペクトルを得る工程、（ｂ）得られた各スペクトル中のピークを、分光学的手法により要素ピークに分解し、その中の水分子の要素ピークを多変量解析して、被検体の解析モデルを作成する工程、および、（ｃ）未知の被検体を、上記工程（ａ）の光の照射および上記工程（ｂ）の分光学的手法に供して、その水分子の要素ピークのスペクトルパターンから、未知の被検体を同定する工程、を含む、方法。

(12) 被検体が、天然物、人工物およびそれらの加工品から選ばれる、上記(11)記載の方法。

(13) 被検体が、生体（ヒトを除く）、農産物およびその加工品、畜産物およびその加工品、並びに海産物およびその加工品から選ばれる、上記(11)記載の方法。

(14) 多変量解析が主成分分析である、上記(11)記載の方法。

(15) 分光学的手法が２次微分処理である、上記(11)記載の方法。

(16) （ａ）被検体に、定期的に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、被検体の複数のスペクトルを得る工程、（ｂ）得られた各スペクトル中のピークを、分光学的手法により要素ピークに分解する工程、および、（ｃ）それらの水分子の要素ピークのスペクトルパターンから、当該被検体における経時変化をリアルタイムでモニターする工程、を含む、方法。

(17) 被検体が、天然物、人工物およびそれらの加工品から選ばれる、上記(16)記載の方法。

(18) 被検体が、生体（ヒトを除く）、農産物およびその加工品、畜産物およびその加工品、並びに海産物およびその加工品から選ばれる、上記(16)記載の方法。

(19) 分光学的手法が２次微分処理である、上記(16)記載の方法。

【０００９】

【発明の実施の形態】以下、本発明を詳細に説明する。本発明においては、まず、被検体に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を

照射して、被検体のスペクトルを得る。

【００１０】本発明において、「４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光」とは、４００ｎｍ～２５００ｎｍの範囲またはその一部の範囲（例えば６００～１０００ｎｍ）の、その範囲全体にわたって連続的に波長を変化させた光をいい、例えば、６００ｎｍから１０００ｎｍまで１ｎｍずつ波長を連続的に変化させた光である。

【００１１】本発明で用いられる近赤外線分光光度計としては、特に制限なく、公知の近赤外線分光光度計が使用できる。

【００１２】次いで、得られたスペクトル中のピークを、分光学的手法により要素ピークに分解する。本発明において、要素ピークに分解する分光学的手法としては、例えば、２次微分処理、フーリエ変換、ウェブレット変換、ニューラルネットワーク法等が例示されるが、本発明はこれらには限定されず、公知の分光学的手法および本発明以降の新たな分光学的手法も全て本発明に含まれる。また、被検体情報の分析に必要とされる分光学的手法が選択して用いられる。

【００１３】モデルを作成する場合には、次に、上記要素ピーク中の水分子の要素ピークを多変量解析する。本発明で使用できる多変量解析としては、主成分分析、因子分析、クラスター分析、ＳＩＭＣＡ（soft independent modeling of class analogy）等が例示されるが、本発明はこれらには限定されず、公知の多変量解析法および本発明以降の新たな多変量解析法も全て本発明に含まれる。また、被検体情報の分析に必要とされる多変量解析法が選択して用いられる。

【００１４】上記の中でも、より現実的な予測機能がある点で、ＳＩＭＣＡを用いることが好ましい。ＳＩＭＣＡは群毎の主成分分析であり、未知の被検体が、どのクラスに属するかあるいは属さないかを判別できる。

【００１５】具体的には、群毎に被検体の水分子の要素ピークを主成分分析して、互いに無相関な複数の主成分に情報を要約し、これらの主成分スコアの分布に基づいて、群毎に主成分モデルを作成する。そして、未知の被検体がどの群に属するかあるいは属さないかを、ＳＩＭＣＡにより判別する。

【００１６】水は その物理化学的特性が極めて特異的であり、これは 水分子の水素結合状態によるものと考えられている。水分子の水素結合状態は９種類あることが知られており、それらは５種に分類されることも知られている。また、９７０ｎｍ近傍の水分子のピークは、水素結合状態が異なる５種の水分子の要素ピークに分解されることも知られている。

【００１７】水においては、水分子同士が水素結合している。ここに他の成分が加わると、水分子間の水素結合に切断が生じたり、水分子と他の成分との間で新たな水素結合が形成される等、水素結合状態は変化する。被検体はたいていの場合、多量の水を含有し、かつ水以外の他の構成成分も含有する。

【００１８】本発明者は、可視－近赤外スペクトル中のピークを分光学的手法により要素ピークに分解し、その中の水分子の要素ピークと、水分子と他の成分との水素結合状態との関係を鋭意研究した結果、水分子と他の成分との相互作用（水素結合状態の変化）により、水分子の要素ピークがシフトしたり、強度が変化するという知見を得た。

【００１９】本発明者は、水と、水にラクトース、ＮａＣｌまたはアルブミンを添加したものについて、それぞれ、６００～１０００ｎｍの近赤外線を照射し、スペクトル中のピークを分光学的手法により要素ピークに分解し、その中の水分子の要素ピークを主成分分析した。そのときの第１および第２主成分ローディングを図１～４に示す。また、このローディングで示される水分子の要素ピークを表１に示す。ここでは、５．２６ｇ／ｍｌのラクトース水溶液、１．２７ｇ／ｍｌのＮａＣｌ水溶液、２．５６ｇ／ｍｌのアルブミン水溶液について上記の方法でそれぞれスペクトルを得、その後これらの溶液を２倍希釈して、同様にそれぞれスペクトルを得、さらに２倍希釈して、同様にそれぞれスペクトルを得る、というように繰り返して、ラクトース水溶液、ＮａＣｌ水溶液、アルブミン水溶液について、それぞれ１５のスペクトルを得、これらを上記方法で要素ピークに分解し、その中の水分子の要素ピークを主成分分析した。

【００２０】なお、近赤外スペクトルの測定には、近赤外分光光度計（Fantoc社（株）製、FRUIT　TESTER20、セル長１ｍｍ）を使用して、６００～１０００ｎｍの近赤外線を照射（６００ｎｍから１０００ｎｍまで１ｎｍ間隔で）した。得られたスペクトルＴを吸光度スペクトルに変換するためにｌｏｇ（１／Ｔ）を計算し、次いでスムージング処理した。次いで、スペクトル中のピークを２次微分処理して要素ピークに分解し、その中の水分子の要素ピークを主成分分析した。これらの一連の処理には、データ処理ソフトとして、Pirouette2.6（GLサイエンス社（株）製）を使用した。

【００２１】

【表１】

Water	Water(W)	Water(W)	Water(W)
	W + Lact	W + NaCl	W + Alb
619nm			
624		622	
628		630	
638			
		648	
652	656	654	654
662		664	
	676	676	
690	690	690	694
704		708	
716			
724			
	730	730	728
740		740	
748	744		
760	760	762	762
770			
782	780	780	778
794	796	798	796
810	810		
814		814	815
		828	
830	838		834
842		840	
858			
872			
874	876	876	876
888		890	
898			
914	908	910, 914	916
924	932	932	932
946			
	952	950	938
964	962	968	968
	974		
984		972	
	992		

【００２２】表１より、水にラクトース、ＮａＣｌまたはアルブミンを添加したものにおいては、それらの水分子の要素ピークが、水単独における水分子の要素ピークと比べてシフトしていることがわかる。

【００２３】例えば、代表的には、水単独における水分子の要素ピーク６５２ｎｍ、７２４ｎｍ、７４０ｎｍ、７８２ｎｍ、７９４ｎｍ、８４２ｎｍ、８７２ｎｍ、９３４ｎｍ、９６４ｎｍは、水にラクトースを添加したものにおいては、それぞれ６５６ｎｍ、７３０ｎｍ、７４４ｎｍ、７８０ｎｍ、７９６ｎｍ、８３８ｎｍ、８７８ｎｍ、９３２ｎｍ、９６２ｎｍにシフトしていることがわかる。

【００２４】また、代表的には、水単独における水分子の要素ピーク６２４ｎｍ、６２８ｎｍ、６５２ｎｍ、６６２ｎｍ、７０４ｎｍ、７２４ｎｍ、７６０ｎｍ、７８２ｎｍ、７９４ｎｍ、８３０ｎｍ、８４２ｎｍ、８７２ｎｍ、８８６ｎｍ、９３４ｎｍ、９６４ｎｍは、水にＮａＣｌを添加したものにおいては、それぞれ６２２ｎｍ、６３０ｎｍ、６５４ｎｍ、６６４ｎｍ、７０８ｎｍ、７３０ｎｍ、７６２ｎｍ、７８０ｎｍ、７９８ｎｍ、８２８ｎｍ、８４６ｎｍ、８７６ｎｍ、８９０ｎｍ、９３２ｎｍ、９６８ｎｍにシフトしていることがわかる。

【００２５】さらに、代表的には、水単独における水分子の要素ピーク６５２ｎｍ、６９０ｎｍ、７２４ｎｍ、７６０ｎｍ、７８２ｎｍ、７９４ｎｍ、８１４ｎｍ、８３０ｎｍ、８７４ｎｍ、９３４ｎｍ、９６４ｎｍは、水にアルブミンを添加したものにおいては、それぞれ６５４ｎｍ、６９４ｎｍ、７２８ｎｍ、７６２ｎｍ、７７８ｎｍ、７９６ｎｍ、８１６ｎｍ、８３４ｎｍ、８７６ｎｍ、９３２ｎｍ、９６８ｎｍにシフトしていることがわかる。

【００２６】このように、他の成分の添加（存在）により水素結合状態が変化すると、スペクトル中の水分子の要素ピークはシフトする（または強度が変化する）。被検体中に存在する水以外の他の構成成分（被検体中の水以外の全成分をいう）の種類および量は個々の被検体により異なり、よって、被検体中の水分子と他の構成成分との水素結合状態は被検体に固有である。従って、被検体中の水と他の構成成分との水素結合状態により変化し得る（シフトし得るまたは強度が変化し得る）この水分子の要素ピークを、被検体に固有の水分子の要素ピークとしてとらえることができる。このような固有の水分子の要素ピークを通して、より高い精度で簡単に被検体の情報を得ることが可能となる。

【００２７】具体的には、より精度の高い解析モデルを作成でき、この解析モデルから、より高い精度で、未知の被検体が属する群の判別や未知の被検体の同定が可能となる。また、水分子の要素ピークのスペクトルパターンから、被検体における情報の経時変化をリアルタイムでモニターすることも可能となる。

【００２８】本発明における被検体としては、特に制限はないが、好ましくは非破壊分析を必要とするものであり、天然物、人工物およびそれらの加工品のいずれでもよい。具体的には、生体（ヒトを除く、牛、マウス等の哺乳動物、魚類、植物等）、農産物（穀類、野菜、豆類、種子類等）またはそれらの加工品、畜産物（牛乳、肉類等）またはそれらの加工品、海産物またはそれらの加工品、土壌、木材、医薬品等が挙げられる。

【００２９】本発明における定性的な情報としては、例

えば、以下のものが挙げられる。
1．被検体がどのグループに属するかを判別する。例えば、被検体の正常・異常を判別する。具体的には、例えば、生体（ヒトを除く）が異常（例えばガン、炎症等の疾病）か正常かを判別する。また、被検体の産地を判別する。具体的には、香料、大豆、小麦等の産地を判別する。さらに、類縁種間の被検体を判別する。具体的には、黒豚由来の肉かその他の豚由来の肉かを判別する。さらに、被検体の等級を判別する。具体的には、水産物、農産物の鮮度により等級を判別する。さらに、被検体があるレベルの品質を有するかどうかを判別する。具体的には、食品加工時にたんぱく質が受けた加熱変性の度合いにより、品質を判別する。
【００３０】具体的な判別方法は、次の手順により行われる。まず、複数の被検体からなる特定の群（例えば、正常・異常別、産地別、種別、等級別、品質別）に属する各被検体に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、各被検体のスペクトルを得る。
【００３１】次いで、得られた各スペクトル中のピークを、分光学的手法（例えば、２次微分処理）により要素ピークに分解し、その中の水分子の要素ピークを多変量解析（例えば、主成分分析）し、そしてそれらの群の解析モデル（例えば、主成分モデル）を作成する。
【００３２】次いで、未知の被検体を、上記と同様の光の照射と分光学的手法に供して、その水分子の要素ピークのスペクトルパターンから、未知の被検体が属する群を判別する。具体的には、その水分子の要素ピークのスペクトルパターンと各群のモデルとの距離から、ＳＩＭＣＡにより判別する。このようにして、例えば、産地、種、等級、品質、個体、正常・異常を識別できる。
【００３３】２．個体（個々の被検体）を同定する。例えば、個々の生体（例えば牛）を同定する。この方法では、人間における指紋のような、個々の生体に固有の情報により、例えば個々の牛にいちいち札をつけることなく管理できる。また、個々の被検体の由来も同定できる。例えば、個々の牛肉、牛乳等の畜産物を同定すれば、それが、それぞれどの牛に由来するものであるかも同定できる。
【００３４】具体的な同定方法は、次の手順により行われる。まず、被検体に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、被検体のスペクトルを得る。
【００３５】次いで、得られたスペクトル中のピークを、分光学的手法（例えば、２次微分処理）により要素ピークに分解する。被検体への照射が２回以上である場合、その中の水分子の要素ピークを多変量解析（例えば、主成分分析）して、そして被検体の解析モデル（例えば、主成分モデル）を作成する。被検体への照射が１回のみである場合、水分子の要素ピークのスペクトルパターンを被検体に固有のスペクトルパターンとする。
【００３６】次いで、未知の被検体を、上記と同様の光の照射と分光学的手法に供して、その水分子の要素ピークのスペクトルパターンから、未知の被検体を同定する。具体的には、その水分子の要素ピークのスペクトルパターンと、被検体のモデルとの距離から、ＳＩＭＣＡにより同定する。または、その水分子の要素ピークのスペクトルパターンと、予め得た被検体に固有のスペクトルパターンを比較することにより同定する。
【００３７】３．被検体の経時変化をリアルタイムでモニターする。具体的なモニター方法は、次の手順で行われる。まず、被検体に、定期的に、４００ｎｍから２５００ｎｍまでのまたはその一部の領域の連続波長光を照射して、被検体のスペクトルを得る。
【００３８】次いで、得られた各スペクトル中のピークを、分光学的手法（例えば、２次微分処理）により要素ピークに分解する。そして、それらの水分子の要素ピークのスペクトルパターンから、当該被検体における経時変化をリアルタイムでモニターする。具体的には、各スペクトルパターンを比較し、水分子のどの要素ピークで経時変化が生じた（ピーク強度の変化、ピークの有無等）かを判断する。ここで、１つの要素ピークでの経時変化を見てもよいし、複数の要素ピークでの経時変化を見てもよい。また、上記の全てのスペクトルの水分子の要素ピークを多変量解析（例えば、主成分分析）すると、どの要素ピークに経時変化が生じているか知ることもできる（例えば主成分ローディングから）。このような水分子の要素ピークの経時変化から、被検体に具体的にどのような経時変化が生じているのかを予測することもできる。
【００３９】
【実施例】以下、実施例を挙げて、本発明を具体的に説明するが、本発明はこれらの実施例に限定されるものではない。
【００４０】実施例１：マウスの正常または異常（ガン化）の判別
＜使用動物＞マウス（ＣＤＦ１、雄マウス、日本ＳＬＣより入手、７週齢）に、発ガン性物質であるベンツピレンを添加した飼料（ベンツピレン投与量：０．５ｍｇ／ｋｇ／ｄａｙ）と無添加の飼料とをそれぞれ与えて、温度２５±２℃、湿度６０±３％の条件下で６ヶ月間飼育して、異常マウス群（ベンツピレン投与群、ガン化したマウス群）と正常マウス群（ベンツピレン非投与群）を得、これらを供試した。正常群と異常群（ガン化）の各群を７匹とした。
【００４１】＜スペクトルの測定＞可視－近赤外スペクトルの測定には近赤外分光光度計（Fantoc社（株）製、FRUIT TESTER20）を使用し、正常群および異常群の各マウスについて、マウス全体に、６００～１０００ｎｍの近赤外線を照射（６００ｎｍから１０００ｎｍまで１

ｎｍ間隔で）した。得られた各スペクトルＴを吸光度スペクトルに変換するために、Ｌｏｇ（１／Ｔ）を計算し、そしてスムージング処理した。これらの処理にはデータ処理ソフトとして、Pirouette2.6（GLサイエンス社（株）製）を使用した。

【００４２】＜主成分モデルの作成とマウスの異常の識別＞スムージング処理を行った後、得られた各スペクトル中のピークを、２次微分処理により要素ピークに分解した。次いで、その中の水分子の要素ピークを主成分分析し、抽出した主成分スコアの分布に基づき、各群の主成分モデルを作成した。各群の主成分スコアに基づく分布（第１～３主成分のみ）を図５に示す。図５より、正常群と異常群はそれぞれ１つの群を形成していることがわかる。また、ＳＩＭＣＡにより計算された各群の距離（クラス間距離）を表２に示す。表２より、正常群と異常群の間の距離は１．１５６８であることがわかる。なお、吸光度スペクトルの変換、２次微分処理、主成分分析およびＳＩＭＣＡには、データ処理ソフトとして、Pirouette2.6（GLサイエンス社（株）製）を使用した。

【００４３】

【表２】

	正常マウス群	異常マウス群
正常マウス群	0.0000	1.1563
異常マウス群	1.1568	0.0000

【００４４】上述のマウスのうちの供試しなかったマウスについて、上記と同様の方法により近赤外線照射および２次微分処理を行い、その水分子の要素ピークのスペクトルパターンと各群のモデルとの距離から、ＳＩＭＣＡにより、どの群に属するか、あるいは属さないかを判別した。９０％以上の確率で判別することができた。

【００４５】実施例２：牛乳の同定（牛乳の由来の同定）

＜使用牛乳＞兵庫県立淡路農業技術センターのホルスタイン種牛４匹（ＣＯＷＮｏ．１０５８、ＣＯＷＮｏ．１０６５、ＣＯＷＮｏ．１０６６およびＣＯＷＮｏ．１０７６）由来の牛乳を供試した。各牛乳８～１２サンプルとした。

【００４６】＜スペクトルの測定＞実施例１と同様の方法により、各牛乳について、牛乳に近赤外線を照射してスペクトルを測定し（但し、セル長１ｍｍ）、吸光度スペクトルに変換し、スムージング処理した。

【００４７】＜主成分モデルの作成と牛乳の由来の識別＞スムージング処理を行った後、得られた各スペクトル中のピークを、２次微分処理により要素ピークに分解した。次いで、その中の水分子の要素ピークを主成分分析し、抽出した主成分スコアの分布に基づき、各牛乳の主成分モデルを作成した。各牛乳の主成分スコアに基づく分布（第１主成分および第２主成分のみ）を図６に示す。図６より、各牛乳はそれぞれ１つの群を形成していることがわかる。また、ＳＩＭＣＡにより計算された各牛乳間の距離（クラス間距離）を表３に示す。表３より、各牛乳間の距離は２．９０以上であることがわかる。なお、吸光度スペクトルの変換、スムージング処理、２次微分処理、主成分分析およびＳＩＭＣＡには実施例１と同様のソフトを使用した。

【００４８】

【表３】

	Cow1066	Cow1076	Cow1058	Cow1065
Cow1066	0.0000	3.8969	3.9295	5.4415
Cow1076	3.8939	0.0000	3.2735	2.9085
Cow1058	3.9295	3.2735	0.0000	2.9496
Cow1065	5.4415	2.9085	2.9496	0.0000

【００４９】上記の牛乳中の供試しなかった牛乳について、上記と同様の方法により近赤外線照射および２次微分処理を行い、その水分子の要素ピークのスペクトルパターンと各牛乳のモデルとの距離から、ＳＩＭＣＡにより、どの牛乳であるかを同定した。９０％以上の確率で同定することができた。これにより、その牛乳がどの牛に由来するのか判別することもできた。

【００５０】実施例３：牛の同定

＜使用試料＞兵庫県立淡路農業技術センターのホルスタイン種牛１１匹（ＣＯＷＮｏ．５、ＣＯＷＮｏ．８、ＣＯＷＮｏ．１１、ＣＯＷＮｏ．１２、ＣＯＷＮｏ．１３、ＣＯＷＮｏ．１４、ＣＯＷＮｏ．１５、ＣＯＷＮｏ．２２、ＣＯＷＮｏ．２３、ＣＯＷＮｏ．２４およびＣＯＷＮｏ．７９）を使用し、測定部位は乳房とした。各牛の同じ乳房について３～４回測定した。

【００５１】＜スペクトルの測定＞実施例１と同様の方法により、各牛ごとに、牛の乳房に近赤外線を照射してスペクトルを測定し、吸光度スペクトルに変換し、スムージング処理した。

【００５２】＜主成分モデルの作成と牛の同定＞スムージング処理を行った後、得られた各スペクトル中のピークを、２次微分処理により要素ピークに分解した。次いで、その中の水分子の要素ピークを主成分分析し、抽出した主成分スコアの分布に基づき、各牛の主成分モデルを作成した。各牛の主成分スコアに基づく分布（第１主成分および第２主成分のみ）を図７に示す。図７より、

各牛の主成分モデルはそれぞれ１つの群を形成していることがわかる。また、ＳＩＭＣＡにより計算された各牛間の距離（クラス間距離）を表４に示す。表４より、各牛間の距離は０．９５０７０７以上であることがわかる。なお、吸光度スペクトルの変換、スムージング処理、２次微分処理、主成分分析およびＳＩＭＣＡには実施例１と同様のソフトを使用した。

【００５３】

【表４】

CowNo:	No23	No24	No13	No79	No15	No12	No14	No22	No11	No8	No5
No23	0.000000	4.924523	15.455975	13.107783	9.056864	15.675976	8.217996	4.965828	3.190142	4.378074	2.924453
No24	4.924523	0.000000	21.372469	8.574723	2.019392	8.634310	2.016551	2.367418	2.559258	2.953038	5.102027
No13	15.455975	21.372469	0.000000	15.141356	34.392334	22.388115	23.107071	8.958652	10.958568	12.749018	9.631367
No79	13.107783	8.574723	15.141357	0.000000	17.922415	5.738169	11.460067	3.672505	4.114215	3.506931	12.444767
No15	9.056865	2.019392	34.392334	17.922415	0.000000	20.082096	4.018164	5.588676	3.591189	5.959875	5.674392
No12	15.675976	8.634310	22.388115	5.738169	20.082096	0.000000	10.947310	6.667864	3.405645	2.402924	15.016349
No14	8.217996	2.016551	23.107071	11.460068	4.018164	10.947310	0.000000	4.915682	2.308817	3.475246	6.717184
No22	4.965828	2.367418	8.958653	3.672505	5.588676	6.667864	4.915682	0.000000	3.323818	3.663465	5.074290
No11	3.190142	2.559258	10.958568	4.114215	3.591189	3.405645	2.308816	3.323818	0.000000	0.950707	5.097722
No8	4.378073	2.953038	12.749018	3.506931	5.959875	2.402924	3.475246	3.663465	0.950707	0.000000	6.687946
No5	2.924453	5.102027	9.631366	12.444767	5.674392	15.016348	6.717184	5.074290	5.097722	6.687946	0.000000

【００５４】上記の１１匹中のある牛について、上記と同様の方法により近赤外線照射および２次微分処理を行い、その水分子の要素ピークのスペクトルパターンと各牛のモデルとの距離から、ＳＩＭＣＡにより、どの牛であるかを同定した。９０％以上の確率で同定することができた。

【００５５】実施例４：牛のモニタリング

＜使用試料＞兵庫県立淡路農業技術センターのホルスタイン種牛を使用した。測定部位を乳房とした。

【００５６】実施例１と同様の方法により、搾乳時、３０秒毎に、牛の乳房に近赤外線を照射してスペクトルを測定し、吸光度スペクトルに変換し、スムージング処理した。

【００５７】＜スペクトルパターンの作成と牛のモニタリング＞スムージング処理を行った後、得られた各スペクトル中のピークを、２次微分処理により要素ピークに分解した。なお、吸光度スペクトルの変換、スムージング処理および２次微分処理には実施例１と同様のソフトを使用した。水分子の要素ピークのスペクトルパターン中の、水分子の要素ピーク８４０ｎｍにおける吸光度を図8に示す。図8より、８４０ｎｍにおいて経時変化が生じていることがわかる。

【００５８】

【発明の効果】本発明によれば、可視－近赤外スペクトル中のピークを、分光学的手法により要素ピークに分解し、その中の水分子の要素ピークを通して、非破壊状態で、比較的簡単な装置を用いて、より高い精度で迅速、低コストで、被検体の情報を得ることができる。

【図面の簡単な説明】

【図１】 水のスペクトルの要素ピークを主成分分析した時の第１および第２主成分のローディングを示す図である。

【図２】 水にラクトースを添加したもののスペクトルの要素ピークを主成分分析した時の第１および第２主成分のローディングを示す図である。

【図３】 水にＮａＣｌを添加したもののスペクトルの要素ピークを主成分分析した時の第１および第２主成分のローディングを示す図である。

【図４】 水にアルブミンを添加したもののスペクトルの要素ピークを主成分分析した時の第１および第２主成分のローディングを示す図である。

【図５】 正常マウス群と異常マウス群のスペクトルの要素ピークを主成分分析した時の、主成分スコアに基づく分布を示す図である。

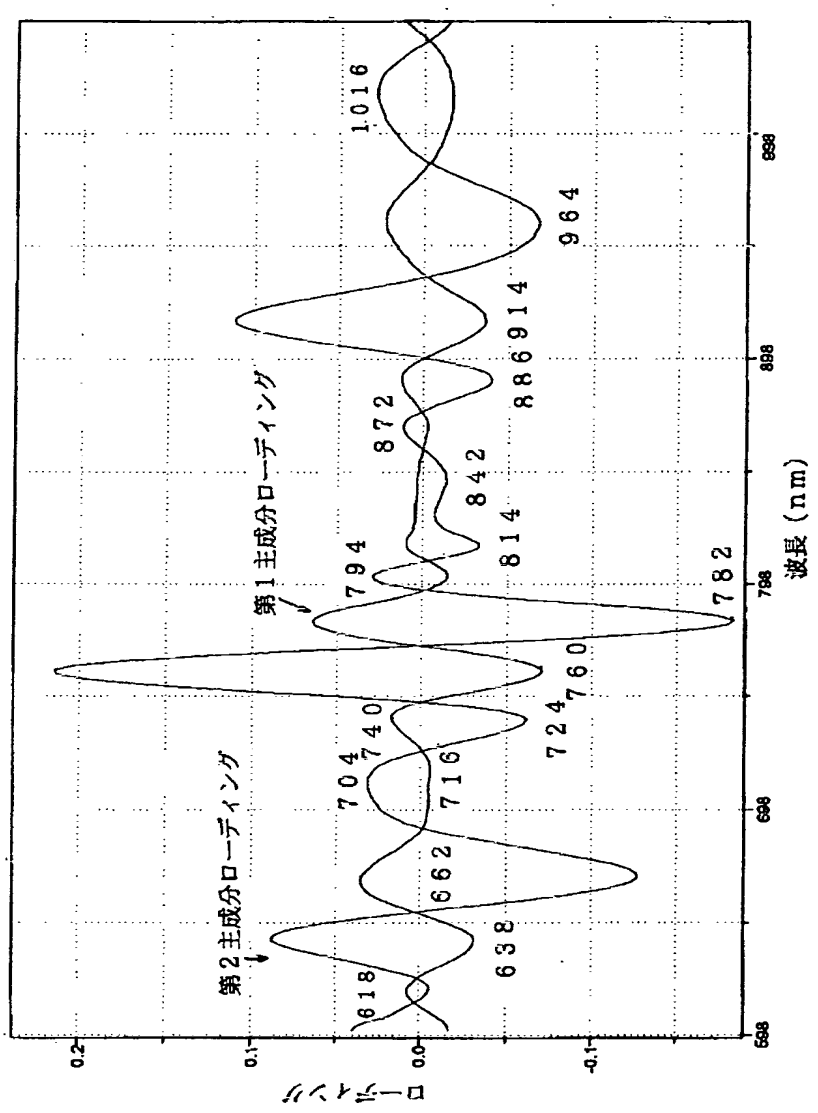
【図６】 由来の異なる牛乳のスペクトルの要素ピークを主成分分析した時の、主成分スコアに基づく分布を示す図である。

【図７】 個々の牛のスペクトルの要素ピークを主成分分析した時の、主成分スコアに基づく分布を示す図である。

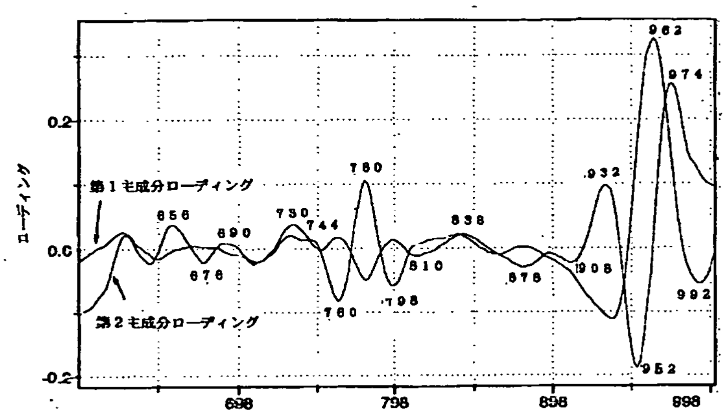
【図８】 牛の乳房のスペクトルを２次微分処理し、その中の水分子の要素ピーク８４０ｎｍにおける吸光度の

経時変化を示す図である。

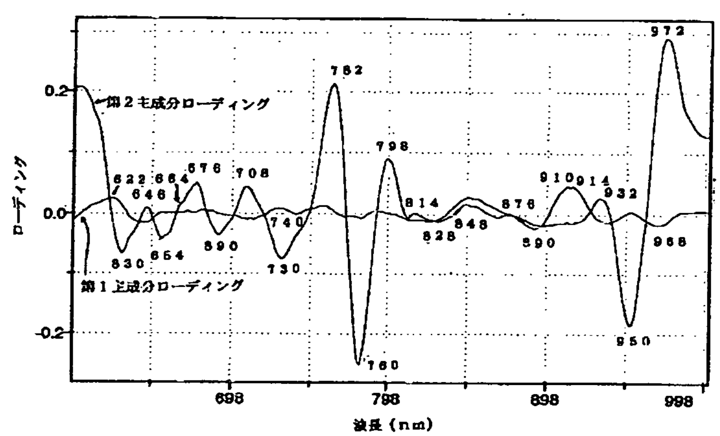
【図1】



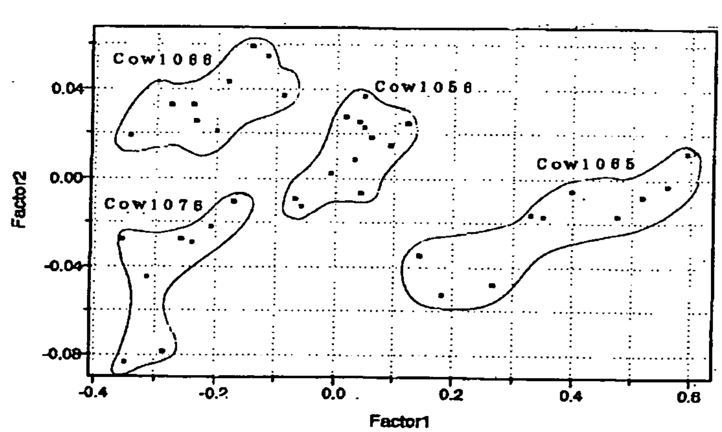
【図2】


962
974
0.2
第1主成分ローディング
760
932
656
730
744
690
838
0.0
676
810
878
908
992
760
798
952
第2主成分ローディング
-0.2
698
798
898
998
ローディング

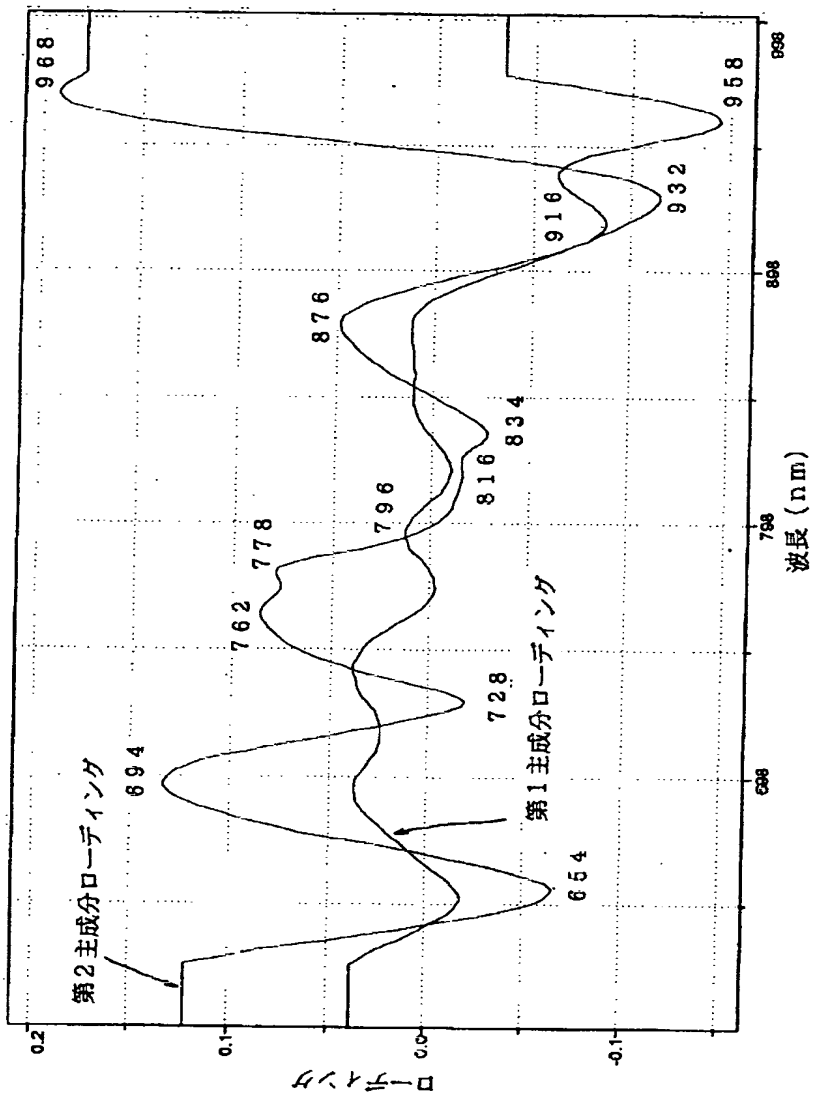
【図3】


972
762
0.2
第2主成分ローディング
798
622
664
676
708
646
814
910
914
932
0.0
740
828
848
876
630
654
690
730
890
968
第1主成分ローディング
-0.2
760
950
698
798
898
998
波長（nm）
ローディング

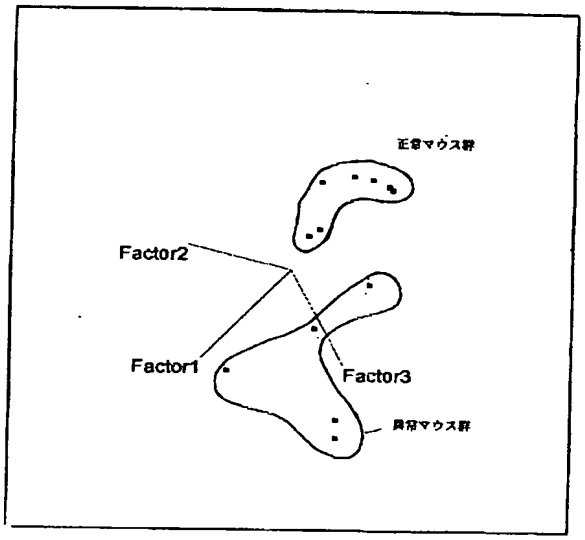
【図6】


Cow1066
Cow1056
Cow1065
Cow1076
0.04
0.00
-0.04
-0.08
Factor2
-0.4
-0.2
0.0
0.2
0.4
0.6
Factor1

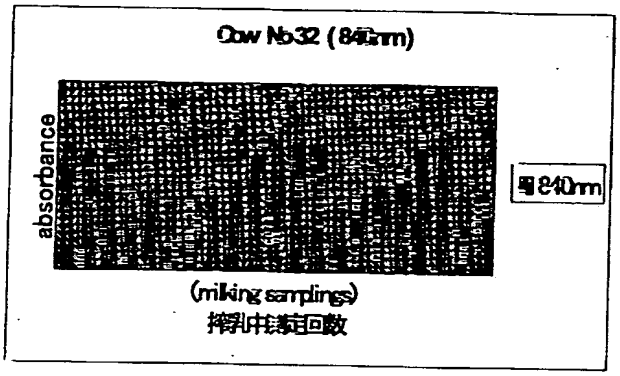
【図4】


968
958
932
916
876
834
816
796
778
762
728
694
654
第2主成分ローディング
第1主成分ローディング
0.2
0.1
0.0
-0.1
698
798
898
998
ローディング
波長（nm）

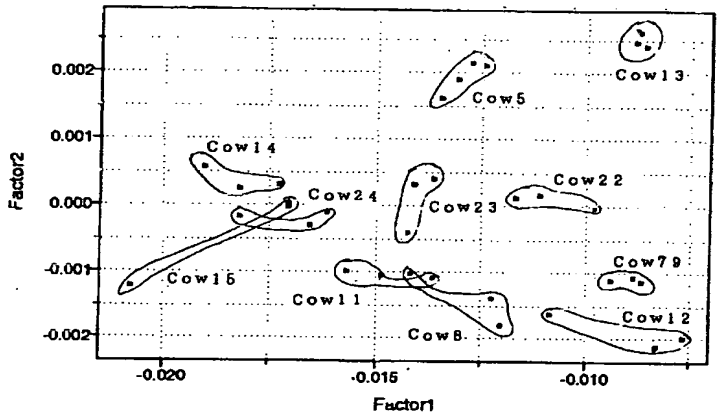
【図５】



【図８】



【図７】



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